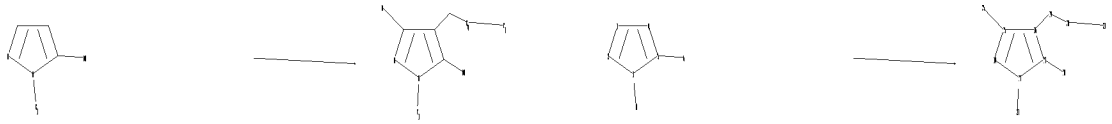
Uploading C:\Program Files\Stnexp\Queries\10594710c.str



chain nodes :
6 8 18 19 20 21 23 25
ring nodes :
1 2 3 4 5 13 14 15 16 17
chain bonds :
1-8 5-6 13-23 15-25 16-19 17-18 19-20 20-21
ring bonds :
1-2 1-5 2-3 3-4 4-5 13-14 13-17 14-15 15-16 16-17
exact/norm bonds :
1-2 1-5 1-8 2-3 3-4 4-5 5-6 13-14 13-17 13-23 14-15 15-16 15-25 16-17
17-18 19-20 20-21
exact bonds :
16-19

G1:H,Cb,Hy,Ak

G2:H,M

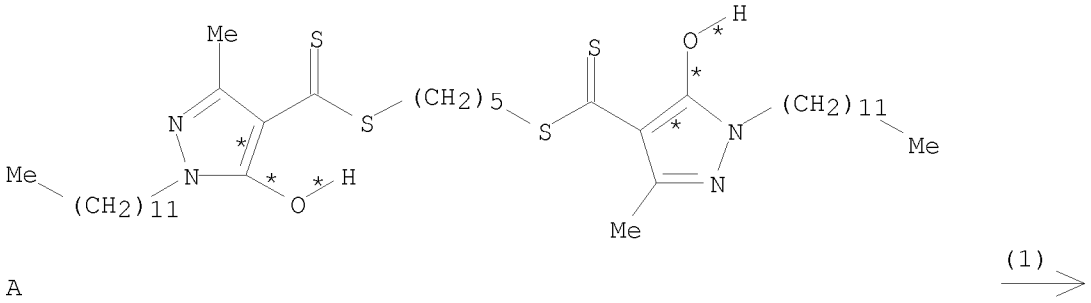
G3:Cb,Hy,Ak

G4:S,SO2

L9 ANSWER 1 OF 3 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 146:242493 CASREACT <<LOGINID::20080928>>
TITLE: Copper(II) complex with the tetradentate ligand 1,5-bis(4-dithiocarboxylate-1-dodecyl-5-hydroxy-3-methylpyrazolyl)pentane. Liquid-liquid extraction study
AUTHOR(S): Oliva, Alfonso; Molinari, Aurora; Avila, Carolina; Flores, Maria Fernanda
CORPORATE SOURCE: Instituto de Quimica, Pontificia Universidad Catolica de Valparaiso, Chile
SOURCE: Journal of the Chilean Chemical Society (2006), 51(2), 865-867
CODEN: JCCSCB; ISSN: 0717-9324
PUBLISHER: Journal of the Chilean Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis of the CuDTC (H2DTC = 1,5-bis(4-dithiocarboxylate-1-dodecyl-

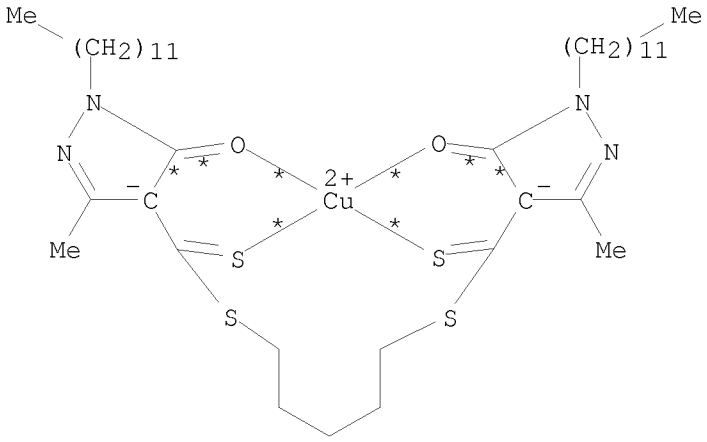
5-hydroxy-3-methylpyrazolyl)pentane) and the solvent extraction behavior of Cu(II) from acid solution (pH 0-5) was studied with the new reagent H2DTC as extractant. The reagent acts as a tetradentate ligand and the extracted species is CuDTC.

RX(1) OF 1 A ===> B



A

(1)



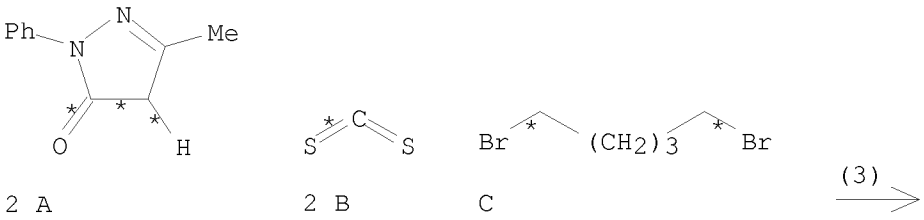
B
YIELD 96%

RX(1) RCT A 856015-09-3
RGT C 142-71-2 Cu(OAc)2
PRO B 924890-66-4
SOL 67-56-1 MeOH, 67-66-3 CHCl3
CON overnight, room temperature
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

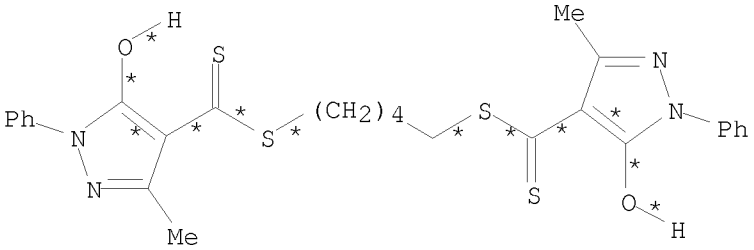
L9 ANSWER 2 OF 3 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 143:78125 CASREACT <<LOGINID::20080928>>
TITLE: 1,5-bis(4-dithiocarboxylate-5-hydroxypyrazolyl)pentane derivatives of 5-pyrazolones
AUTHOR(S): Avila, Carolina; Flores, Maria Fernanda; Molinari,

Aurora; Oliva, Alfonso
CORPORATE SOURCE: Instituto de Quimica, Pontificia Universidad Catolica de Valparaiso, Casilla, 4059, Chile
SOURCE: Journal of Heterocyclic Chemistry (2005), 42(4), 595-597
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 3-Methyl-1-phenyl-2-pyrazolin-5-one and 1-dodecyl-3-methyl-2-pyrazolin-5-one react with carbon disulfide and 1,5-dibromopentane in the presence of sodium acetate in DMF or n-butyllithium in THF to afford 1,5-bis(4-dithiocarboxylate-5-hydroypyrazolyl)pentane derivs.

RX(3) OF 4 2 A + 2 B + C ===> I



2 A 2 B C



I
YIELD 71%

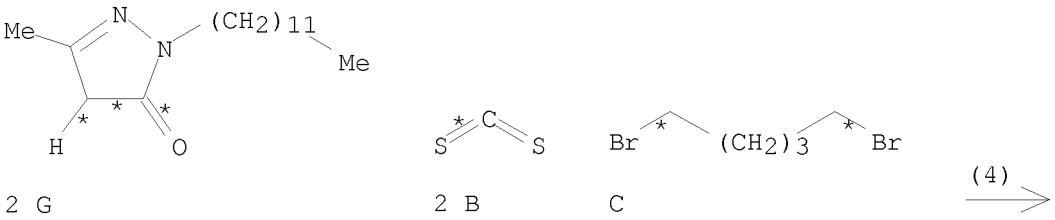
RX(3) RCT A 89-25-8, B 75-15-0

STAGE(1)
RGT E 127-09-3 AcONa
SOL 68-12-2 DMF
CON SUBSTAGE(1) 2 hours, 40 deg C
SUBSTAGE(2) 2 hours, 40 deg C

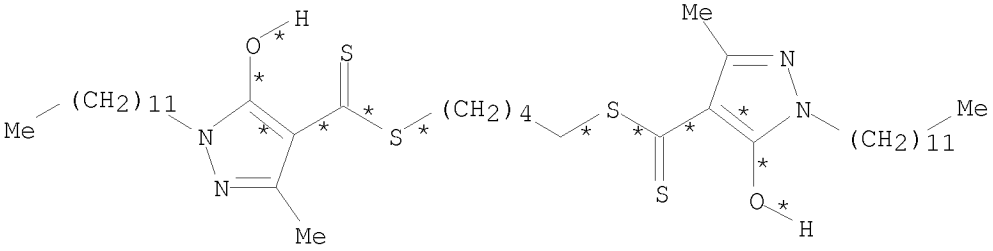
STAGE(2)
RCT C 111-24-0
CON overnight, 40 deg C

PRO I 856015-08-2
NTE similar results were obtained using BuLi/THF/0C in place of NaOAc/DMF/40C

RX(4) OF 4 2 G + 2 B + C ===> J



2 G 2 B C



J
YIELD 77%

RX(4) RCT G 129803-83-4, B 75-15-0

STAGE(1)
RGT E 127-09-3 AcONa
SOL 68-12-2 DMF
CON SUBSTAGE(1) 2 hours, 40 deg C
SUBSTAGE(2) 2 hours, 40 deg C

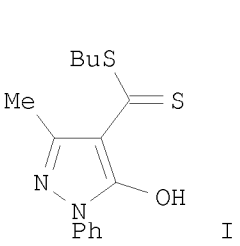
STAGE(2)
RCT C 111-24-0
CON overnight, 40 deg C

PRO J 856015-09-3
NTE similar results were obtained using BuLi/THF/0C in place of NaOAc/DMF/40C

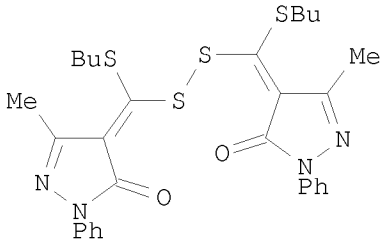
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 3 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 134:71525 CASREACT <<LOGINID::20080928>>
TITLE: Electrosynthesis of a bis-ketene dithioacetal disulfide derivative from 1-phenyl-3-methyl-4-(butyl dithiocarboxylate)-5-pyrazolone using a glassy carbon electrode
AUTHOR(S): Oliva, Alfonso; Molinari, Aurora; Angulo, Jean; Schrebler, Ricardo; Gomez, Humberto; Cordova, Ricardo
CORPORATE SOURCE: Instituto de Quimica, Universidad Catolica de

Valparaiso, Valparaiso, Chile
SOURCE: Synthetic Communications (2000), 30(23), 4353-4360
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



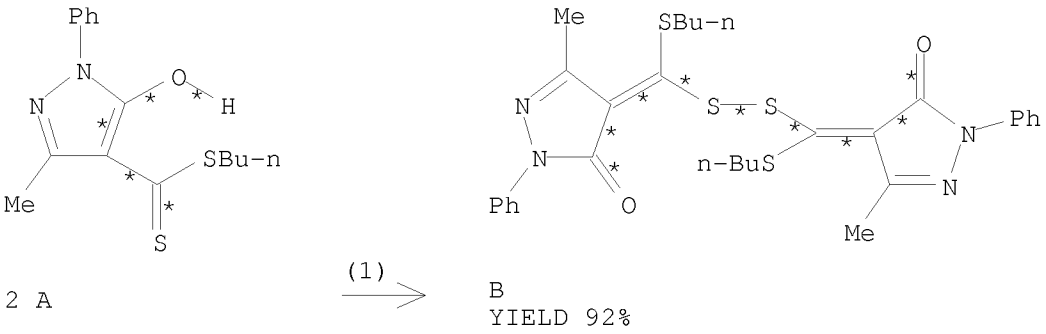
I



II

AB The electrooxidn. of pyrazolone dithio ester I was studied in ethanol-water solution, using a glassy carbon electrode surface. The electrochem. and spectroscopic data are in agreement with bis-ketene dithioacetal disulfide II as the only product.

RX(1) OF 1 2 A ===> B

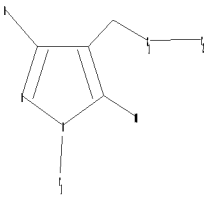


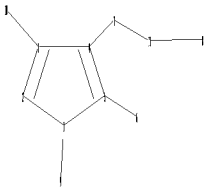
2 A

B
YIELD 92%

RX(1) RCT A 128202-98-2
RGT C 7447-41-8 LiCl
PRO B 314281-72-6
SOL 64-17-5 EtOH, 7732-18-5 Water
NTE electrochem.
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Uploading C:\Program Files\Stnexp\Queries\10594710e.str





chain nodes :
6 7 8 9 10 13
ring nodes :
1 2 3 4 5
chain bonds :
1-9 3-10 4-7 5-6 7-13 8-13
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-9 2-3 3-4 3-10 4-5 5-6 7-13 8-13
exact bonds :
4-7

G1:H,Cb,Cy,Hy,Ak

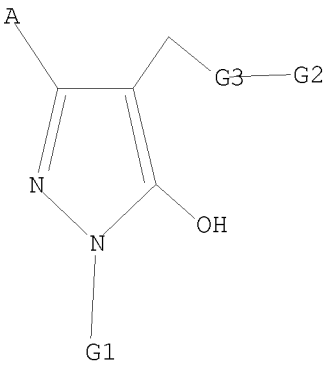
G2:Cb,Cy,Hy,Ak

G3:S,SO2

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
13:CLASS

L10 STRUCTURE UPLOADED

=> d
L10 HAS NO ANSWERS
L10 STR



G1 H,Cb,Cy,Hy,Ak

G2 Cb,Cy,Hy,Ak

G3 S,SO2

Structure attributes must be viewed using STN Express query preparation.

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=> s l10 full
FULL SEARCH INITIATED 19:21:54 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     9869 TO ITERATE

100.0% PROCESSED     9869 ITERATIONS                                68 ANSWERS
SEARCH TIME: 00.00.01

L11          68 SEA SSS FUL L10

=> d l11 1-10

L11  ANSWER 1 OF 68  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   1006311-39-2  REGISTRY
ED   Entered STN:  03 Mar 2008
CN   1H-Pyrazole-4-carbodithioic acid, 5-hydroxy-3-methyl-1-(4-methylphenyl)-,
     propyl ester  (CA INDEX NAME)
MF   C15 H18 N2 O S2
SR   Chemical Library
       Supplier: Aurora Fine Chemicals
LC   STN Files:   CHEMCATS
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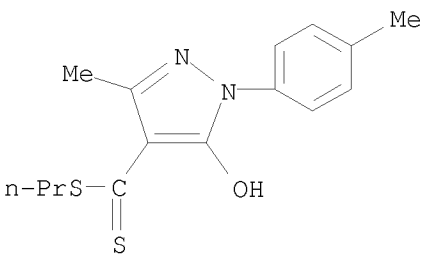
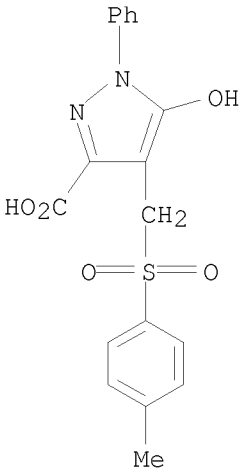


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

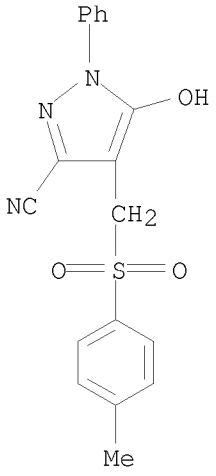
L11 ANSWER 2 OF 68 REGISTRY COPYRIGHT 2008 ACS on STN
RN 866496-21-1 REGISTRY
ED Entered STN: 01 Nov 2005
CN 1H-Pyrazole-3-carboxylic acid, 5-hydroxy-4-[[(4-methylphenyl)sulfonyl]methyl]-1-phenyl- (CA INDEX NAME)
MF C18 H16 N2 O5 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

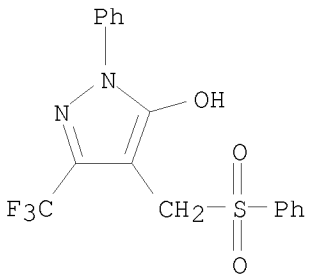
L11 ANSWER 3 OF 68 REGISTRY COPYRIGHT 2008 ACS on STN
RN 866496-20-0 REGISTRY
ED Entered STN: 01 Nov 2005
CN 1H-Pyrazole-3-carbonitrile, 5-hydroxy-4-[[(4-methylphenyl)sulfonyl]methyl]-1-phenyl- (CA INDEX NAME)
MF C18 H15 N3 O3 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L11 ANSWER 4 OF 68 REGISTRY COPYRIGHT 2008 ACS on STN
RN 866496-17-5 REGISTRY
ED Entered STN: 01 Nov 2005
CN 1H-Pyrazol-5-ol, 1-phenyl-4-[(phenylsulfonyl)methyl]-3-(trifluoromethyl)-
(CA INDEX NAME)
MF C17 H13 F3 N2 O3 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

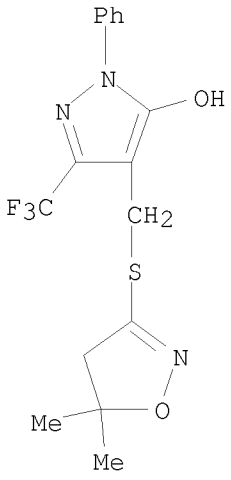


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L11 ANSWER 5 OF 68 REGISTRY COPYRIGHT 2008 ACS on STN
RN 866496-16-4 REGISTRY
ED Entered STN: 01 Nov 2005
CN 1H-Pyrazol-5-ol, 4-[[(4,5-dihydro-5,5-dimethyl-3-isoxazolyl)thio]methyl]-1-
phenyl-3-(trifluoromethyl)- (CA INDEX NAME)
MF C16 H16 F3 N3 O2 S

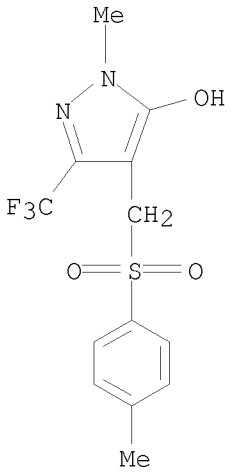
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

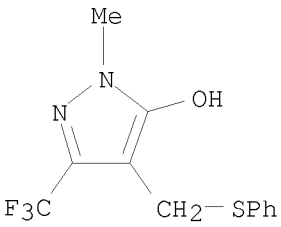
L11 ANSWER 6 OF 68 REGISTRY COPYRIGHT 2008 ACS on STN
RN 866496-15-3 REGISTRY
ED Entered STN: 01 Nov 2005
CN 1H-Pyrazol-5-ol, 1-methyl-4-[[(4-methylphenyl)sulfonyl]methyl]-3-(trifluoromethyl)- (CA INDEX NAME)
MF C13 H13 F3 N2 O3 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

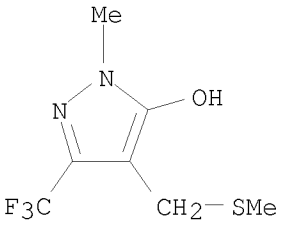
L11 ANSWER 7 OF 68 REGISTRY COPYRIGHT 2008 ACS on STN
RN 866496-14-2 REGISTRY
ED Entered STN: 01 Nov 2005
CN 1H-Pyrazol-5-ol, 1-methyl-4-[(phenylthio)methyl]-3-(trifluoromethyl)- (CA INDEX NAME)
MF C12 H11 F3 N2 O S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L11 ANSWER 8 OF 68 REGISTRY COPYRIGHT 2008 ACS on STN
RN 866496-13-1 REGISTRY
ED Entered STN: 01 Nov 2005
CN 1H-Pyrazol-5-ol, 1-methyl-4-[(methylthio)methyl]-3-(trifluoromethyl)- (CA INDEX NAME)
MF C7 H9 F3 N2 O S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

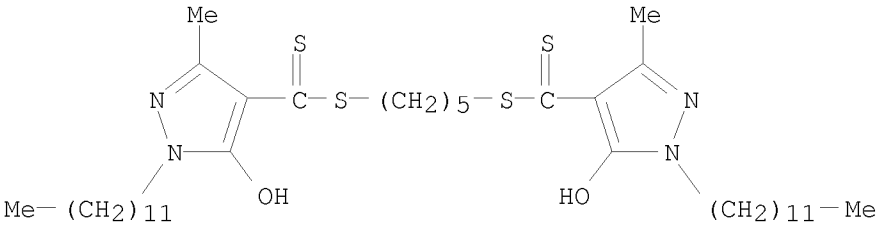


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L11 ANSWER 9 OF 68 REGISTRY COPYRIGHT 2008 ACS on STN
RN 856015-09-3 REGISTRY

ED Entered STN: 19 Jul 2005
CN 1H-Pyrazole-4-carbodithioic acid, 1-dodecyl-5-hydroxy-3-methyl-,
    S,S'-1,5-pentanediyl ester (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1H-Pyrazole-4-carbodithioic acid, 1-dodecyl-5-hydroxy-3-methyl-,
    1,5-pentanediyl ester (9CI)
MF C39 H68 N4 O2 S4
SR CA
LC STN Files: CA, CAPLUS, CASREACT



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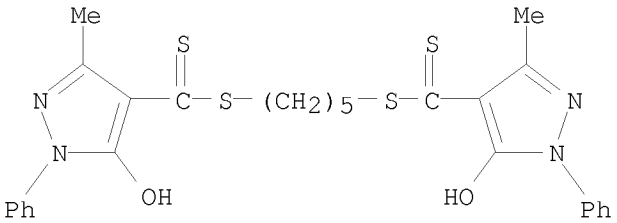
              2 REFERENCES IN FILE CA (1907 TO DATE)
              2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L11 ANSWER 10 OF 68 REGISTRY COPYRIGHT 2008 ACS on STN
RN 856015-08-2 REGISTRY
ED Entered STN: 19 Jul 2005
CN 1H-Pyrazole-4-carbodithioic acid, 5-hydroxy-3-methyl-1-phenyl-,
    1,5-pentanediyl ester (9CI) (CA INDEX NAME)
MF C27 H28 N4 O2 S4
SR CA
LC STN Files: CA, CAPLUS, CASREACT



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

              1 REFERENCES IN FILE CA (1907 TO DATE)
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=> S L12

L13   2 L12

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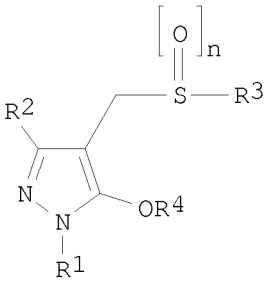
L13 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1200395 CAPLUS <<LOGINID::20080928>>
DOCUMENT NUMBER: 143:460143
TITLE: Process for the preparation of 5-difluoromethoxy-4-thiomethylpyrazoles via fluoroalkylation
INVENTOR(S): Uchida, Yukio
PATENT ASSIGNEE(S): Ihara Chemical Industry Co., Ltd., Japan
SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005105755	A1	20051110	WO 2005-JP7847	20050425
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2007246396	A	20070927	JP 2004-132764	20040428
PRIORITY APPLN. INFO.:			JP 2004-132764 A	20040428

OTHER SOURCE(S): MARPAT 143:460143
GI



I

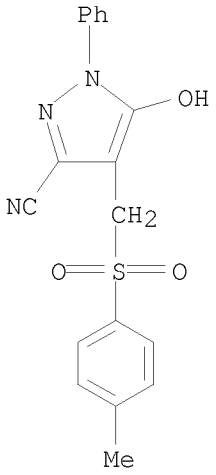
AB A process for the preparation of compound I [R1 = alkyl, (un)substituted aromatic hydrocarbon, (un)substituted heterocycle; R2 = electron withdrawing group; R3 = alkyl, (un)substituted aromatic hydrocarbon, (un)substituted heterocycle; R4 = CHF2; n = 0, 2], characterized by reaction of compds. I [R1, R2, R3, n = same as above; R4 = H] with F2CHX [X = halo] in the presence of sodium hydroxide in dialkyl ketone or alkyl nitrile, was provided. For example, a solution of 3-[(5-hydroxy-1-phenyl-3-

trifluoromethylpyrazol-4-yl)methylthio]-4,5-dihydro-5,5-dimethylisoxazole (33.2 g) and NaOH (12.0 g) in acetonitrile (100 mL) was stirred at room temperature for 1 h. To the resulting mixture was added chlorodifluoromethane (17.3 g) over a period of 4 h, while maintaining the reaction temperature between 5-15 °C. The reaction was stirred for 5 h, followed by work-up and silica-gel purification to afford 3-[(5-difluoromethoxy-1-methyl-3-trifluoromethylpyrazol-4-yl)methylthio]-4,5-dihydro-5,5-dimethylisoxazole (22.6 g).

IT 866496-20-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(thiomethylation of pyrazole compds. using formaldehyde)

RN 866496-20-0 CAPLUS

CN 1H-Pyrazole-3-carbonitrile, 5-hydroxy-4-[[(4-methylphenyl)sulfonyl]methyl]-1-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:1103753 CAPLUS <<LOGINID::20080928>>

DOCUMENT NUMBER: 143:387027

TITLE: Process for preparation of 5-hydroxy-4-thiomethylpyrazole derivatives

INVENTOR(S): Uchida, Yukio

PATENT ASSIGNEE(S): Ihara Chemical Industry Co., Ltd., Japan

SOURCE: PCT Int. Appl., 50 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005095352	A1	20051013	WO 2005-JP6806	20050331

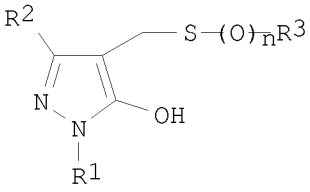
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO,

NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
MR, NE, SN, TD, TG

JP 2005289824	A	20051020	JP 2004-102963	20040331
AU 2005228017	A1	20051013	AU 2005-228017	20050331
CA 2560936	A1	20051013	CA 2005-2560936	20050331
CN 1938278	A	20070328	CN 2005-80010635	20050331
EP 1767528	A1	20070328	EP 2005-728918	20050331
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR				
BR 2005009353	A	20070911	BR 2005-9353	20050331
KR 2007003964	A	20070105	KR 2006-719480	20060921
IN 2006DN05581	A	20070831	IN 2006-DN5581	20060925
MX 2006PA11130	A	20070125	MX 2006-PA11130	20060928
US 20070185334	A1	20070809	US 2006-594710	20060928
PRIORITY APPLN. INFO.:			JP 2004-102963 A	20040331
			WO 2005-JP6806 W	20050331

OTHER SOURCE(S): MARPAT 143:387027

GI



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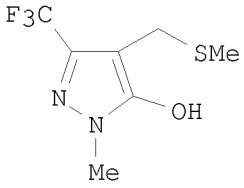


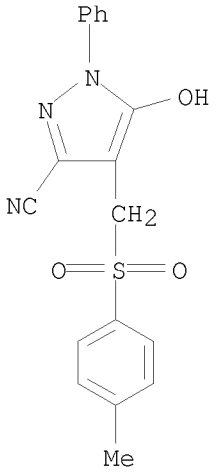
II

AB This invention pertains to a method for producing pyrazole derivs. I [wherein R1 = H, alkyl, (un)substituted hydrocarbyl, or heterocyclyl; R2 = electron withdrawing group; R3 = alkyl, (un)substituted hydrocarbyl, or heterocyclyl; n = 0 or 2]. For example, 5-hydroxy-1-methyl-3-(trifluoromethyl)pyrazole (preparation given) was reacted with 35% formalin in H2O in the presence of NaOH, followed by the addition of NaSMe to give II (72.7%). This process enables the 5-hydroxy-4-thiomethylpyrazole compds. to be easily produced in high yield under mild conditions through a single step without the necessity of using any special apparatus, expensive catalyst, transition metal, etc. It is friendly to the environment because it generates substantially no harmful wastes derived from a catalyst, etc.

IT 866496-20-0P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of 5-hydroxy-4-thiomethylpyrazole derivs.)

RN 866496-20-0 CAPLUS

CN 1H-Pyrazole-3-carbonitrile, 5-hydroxy-4-[[(4-methylphenyl)sulfonyl]methyl]-1-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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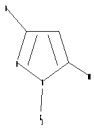

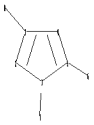

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6 7 8
ring nodes :
1 2 3 4 5
chain bonds :
1-7 3-8 5-6
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-7 2-3 3-4 3-8 4-5 5-6

G1:H,Cb,Cy,Hy,Ak

G2:Cb,Cy,Hy,Ak

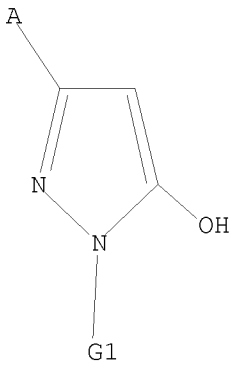
G3:S,SO2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS

L16   STRUCTURE UPLOADED

=> d
L16 HAS NO ANSWERS
L16   STR



G1 H,Cb,Cy,Hy,Ak

G2 Cb,Cy,Hy,Ak

G3 S,SO2

Structure attributes must be viewed using STN Express query preparation.

=> s l16 full
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FULL SCREEN SEARCH COMPLETED -   270331 TO ITERATE

100.0% PROCESSED   270331 ITERATIONS   10523 ANSWERS
SEARCH TIME: 00.00.03

L17   10523 SEA SSS FUL L16

=> s l18 and formaldehyde?
        158420 FORMALDEHYDE?
L19   2 L18 AND FORMALDEHYDE?

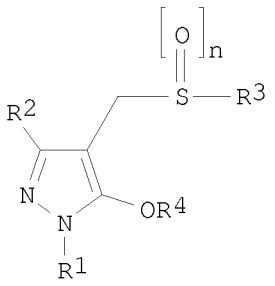
=> d l19 1-2 ibib abs hitstr

L19 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1200395 CAPLUS <<LOGINID::20080928>>
DOCUMENT NUMBER: 143:460143
TITLE: Process for the preparation of 5-difluoromethoxy-4-
                         thiomethylpyrazoles via fluoroalkylation
INVENTOR(S):   Uchida, Yukio
PATENT ASSIGNEE(S):   Ihara Chemical Industry Co., Ltd., Japan
SOURCE: PCT Int. Appl., 27 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005105755	A1	20051110	WO 2005-JP7847	20050425
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2007246396	A	20070927	JP 2004-132764	20040428

PRIORITY APPLN. INFO.: JP 2004-132764 A 20040428
OTHER SOURCE(S): MARPAT 143:460143
GI

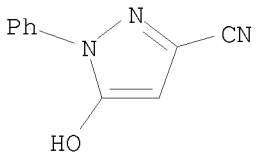


I

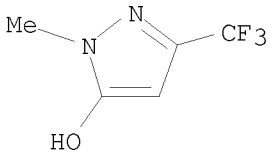
AB A process for the preparation of compound I [R1 = alkyl, (un)substituted aromatic hydrocarbon, (un)substituted heterocycle; R2 = electron withdrawing group; R3 = alkyl, (un)substituted aromatic hydrocarbon, (un)substituted heterocycle; R4 = CHF2; n = 0, 2], characterized by reaction of compds. I [R1, R2, R3, n = same as above; R4 = H] with F2CHX [X = halo] in the presence of sodium hydroxide in dialkyl ketone or alkyl nitrile, was provided. For example, a solution of 3-[(5-hydroxy-1-phenyl-3-trifluoromethylpyrazol-4-yl)methylthio]-4,5-dihydro-5,5-dimethylisoxazole (33.2 g) and NaOH (12.0 g) in acetonitrile (100 mL) was stirred at room temperature for 1 h. To the resulting mixture was added chlorodifluoromethane (17.3 g) over a period of 4 h, while maintaining the reaction temperature between 5-15 °C. The reaction was stirred for 5 h, followed by work-up and silica-gel purification to afford 3-[(5-difluoromethoxy-1-methyl-3-trifluoromethylpyrazol-4-yl)methylthio]-4,5-dihydro-5,5-dimethylisoxazole (22.6 g).

IT 63650-60-2, 3-Cyano-5-hydroxy-1-phenylpyrazole 122431-37-2, 5-Hydroxy-1-methyl-3-trifluoromethylpyrazole
RL: RCT (Reactant); RACT (Reactant or reagent)
(thiomethylation of pyrazole compds. using formaldehyde)

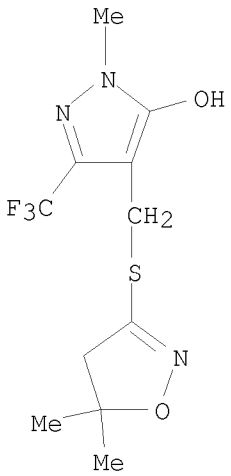
RN 63650-60-2 CAPLUS
CN 1H-Pyrazole-3-carbonitrile, 5-hydroxy-1-phenyl- (CA INDEX NAME)



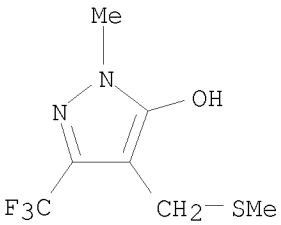
RN 122431-37-2 CAPLUS
CN 1H-Pyrazol-5-ol, 1-methyl-3-(trifluoromethyl)- (CA INDEX NAME)



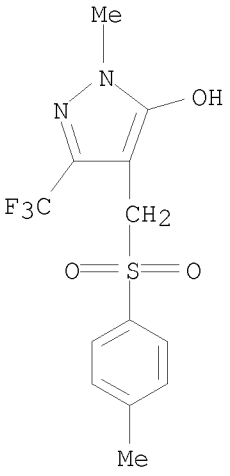
IT 447402-29-1P 866496-13-1P 866496-15-3P
866496-20-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(thiomethylation of pyrazole compds. using formaldehyde)
RN 447402-29-1 CAPLUS
CN 1H-Pyrazol-5-ol, 4-[[(4,5-dihydro-5,5-dimethyl-3-isoxazolyl)thio]methyl]-1-methyl-3-(trifluoromethyl)- (CA INDEX NAME)



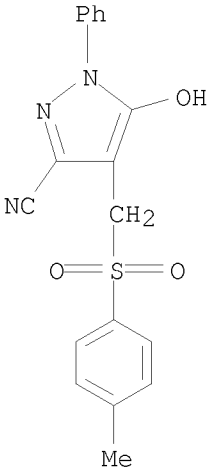
RN 866496-13-1 CAPLUS
CN 1H-Pyrazol-5-ol, 1-methyl-4-[(methylthio)methyl]-3-(trifluoromethyl)- (CA INDEX NAME)



RN 866496-15-3 CAPLUS
CN 1H-Pyrazol-5-ol, 1-methyl-4-[[(4-methylphenyl)sulfonyl]methyl]-3-(trifluoromethyl)- (CA INDEX NAME)



RN 866496-20-0 CAPLUS
CN 1H-Pyrazole-3-carbonitrile, 5-hydroxy-4-[[(4-methylphenyl)sulfonyl]methyl]-1-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1103753 CAPLUS <<LOGINID::20080928>>
DOCUMENT NUMBER: 143:387027
TITLE: Process for preparation of 5-hydroxy-4-thiomethylpyrazole derivatives
INVENTOR(S): Uchida, Yukio
PATENT ASSIGNEE(S): Ihara Chemical Industry Co., Ltd., Japan
SOURCE: PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005095352	A1	20051013	WO 2005-JP6806	20050331
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2005289824	A	20051020	JP 2004-102963	20040331
AU 2005228017	A1	20051013	AU 2005-228017	20050331
CA 2560936	A1	20051013	CA 2005-2560936	20050331
CN 1938278	A	20070328	CN 2005-80010635	20050331
EP 1767528	A1	20070328	EP 2005-728918	20050331
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR				
BR 2005009353	A	20070911	BR 2005-9353	20050331
KR 2007003964	A	20070105	KR 2006-719480	20060921
IN 2006DN05581	A	20070831	IN 2006-DN5581	20060925
MX 2006PA11130	A	20070125	MX 2006-PA11130	20060928
US 20070185334	A1	20070809	US 2006-594710	20060928
PRIORITY APPLN. INFO.:			JP 2004-102963 A	20040331
			WO 2005-JP6806 W	20050331

OTHER SOURCE(S): MARPAT 143:387027
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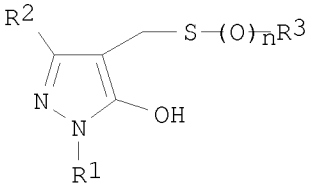

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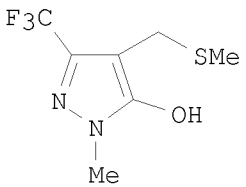

II

AB This invention pertains to a method for producing pyrazole derivs. I

[wherein R1 = H, alkyl, (un)substituted hydrocarbyl, or heterocyclyl; R2 = electron withdrawing group; R3 = alkyl, (un)substituted hydrocarbyl, or heterocyclyl; n = 0 or 2]. For example, 5-hydroxy-1-methyl-3-(trifluoromethyl)pyrazole (preparation given) was reacted with 35% formalin in H2O in the presence of NaOH, followed by the addition of NaSMe to give II (72.7%). This process enables the 5-hydroxy-4-thiomethylpyrazole compds. to be easily produced in high yield under mild conditions through a single step without the necessity of using any special apparatus, expensive catalyst, transition metal, etc. It is friendly to the environment because it generates substantially no harmful wastes derived from a catalyst, etc.

IT 51986-17-5P 63650-60-2P 96145-98-1P
122431-37-2P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of 5-hydroxy-4-thiomethylpyrazole derivs.)

RN 51986-17-5 CAPLUS
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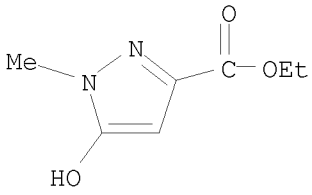
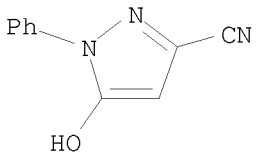
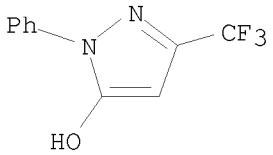


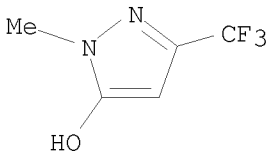
RN 63650-60-2 CAPLUS
CN 1H-Pyrazole-3-carbonitrile, 5-hydroxy-1-phenyl- (CA INDEX NAME)



RN 96145-98-1 CAPLUS
CN 1H-Pyrazol-5-ol, 1-phenyl-3-(trifluoromethyl)- (CA INDEX NAME)

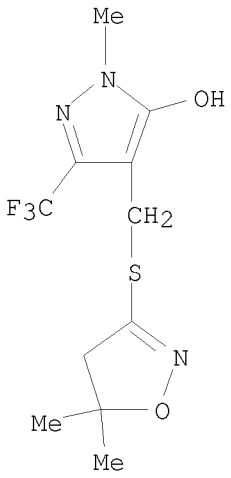


RN 122431-37-2 CAPLUS
CN 1H-Pyrazol-5-ol, 1-methyl-3-(trifluoromethyl)- (CA INDEX NAME)

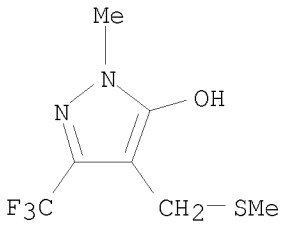


IT 447402-29-1P 866496-13-1P 866496-14-2P
866496-15-3P 866496-16-4P 866496-17-5P
866496-20-0P 866496-21-1P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of 5-hydroxy-4-thiomethylpyrazole derivs.)

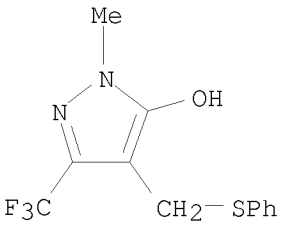
RN 447402-29-1 CAPLUS
CN 1H-Pyrazol-5-ol, 4-[[(4,5-dihydro-5,5-dimethyl-3-isoxazolyl)thio]methyl]-1-methyl-3-(trifluoromethyl)- (CA INDEX NAME)



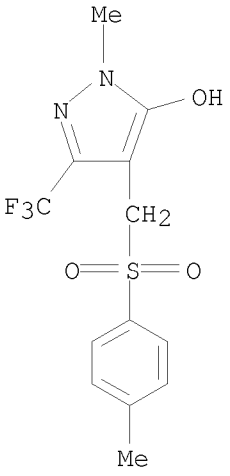
RN 866496-13-1 CAPLUS
CN 1H-Pyrazol-5-ol, 1-methyl-4-[(methylthio)methyl]-3-(trifluoromethyl)- (CA INDEX NAME)



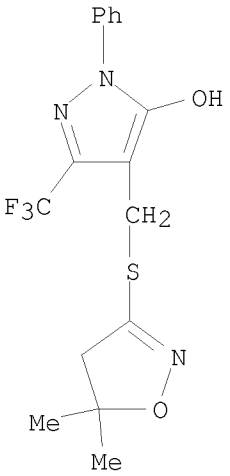
RN 866496-14-2 CAPLUS
CN 1H-Pyrazol-5-ol, 1-methyl-4-[(phenylthio)methyl]-3-(trifluoromethyl)- (CA INDEX NAME)



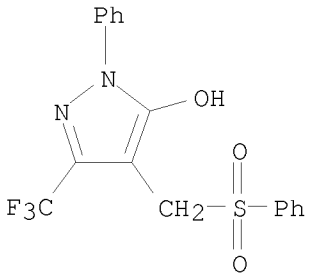
RN 866496-15-3 CAPLUS
CN 1H-Pyrazol-5-ol, 1-methyl-4-[[(4-methylphenyl)sulfonyl]methyl]-3-(trifluoromethyl)- (CA INDEX NAME)



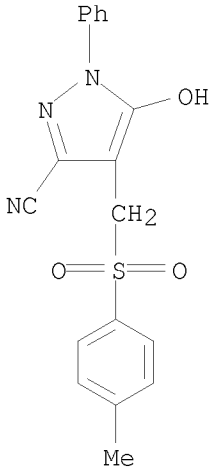
RN 866496-16-4 CAPLUS
CN 1H-Pyrazol-5-ol, 4-[[(4,5-dihydro-5,5-dimethyl-3-isoxazolyl)thio]methyl]-1-phenyl-3-(trifluoromethyl)- (CA INDEX NAME)



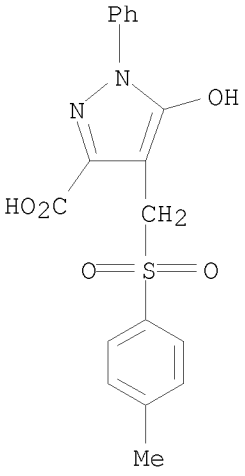
RN 866496-17-5 CAPLUS
CN 1H-Pyrazol-5-ol, 1-phenyl-4-[(phenylsulfonyl)methyl]-3-(trifluoromethyl)-
(CA INDEX NAME)



RN 866496-20-0 CAPLUS
CN 1H-Pyrazole-3-carbonitrile, 5-hydroxy-4-[[(4-methylphenyl)sulfonyl]methyl]-
1-phenyl- (CA INDEX NAME)



RN 866496-21-1 CAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 5-hydroxy-4-[[(4-
methylphenyl)sulfonyl]methyl]-1-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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